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THREE-PARTICLE SCATTERING. II. IN SPACE*

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Abstract

The theory of three-particle collisions in a plane which was developed in an earlier paper is extended to scattering in space. Formal expressions for scattering amplitudes and cross sections are obtained for inelastic and rearrangement collisions as well as for elastic scattering. The optical theorem is also extended to the three-body case. The paper concludes with a discussion of the dynamics of a collision among three structureless particles which interact via a short-range potential. Author

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FIGURE CAPTION

Figure 1. Three-body scattering diagrams. (a) Diagram corresponding to the first-order term in the Born series which contains the interaction V_{12}. This pseudo three-body process is represented by the amplitude given in Eq. (37). (b) and (c) Diagrams corresponding to the second order term in the Born series which contain V_{12} V_{23} and V_{13} V_{12}, respectively. (d) Pseudo three-body diagram corresponding to the second order term in the Born series which contains V_{12} V_{12}.

I INTRODUCTION

In an earlier paper[1] we discussed the scattering of three particles constrained to motion in a plane with the aid of the integral equation of Lippmann and Schwinger.[2 3 4] In the present paper we shall extend this formalism to motion in space, and utilize the results in a simple application.

We found in Paper I that the generalized angular momentum was especially appropriate for treating three-particle collisions in a plane by means of the representations[5] which employ, in addition to the energy K, the dynamical variables

(A) Λ^2, L, and Σ_t

(B) Λ^2, L, and Y

(C) Λ^2, L_1, and L_2

where Λ^2, L, Σ_t, Y, L_1, and L_2 are defined in Eqs. (1) and (5) of Paper I. Although no spatial analogue of (A) has yet been developed, the planar representations (B) and (C) are analogous, respectively, to the following:

(B') Λ^2, L, L_1, L_2, and L_z

(C') Λ^2, L_1, L_2, L_{1_z}, and L_{2_z}

where the L_z are the z-components of ordinary angular momentum. It is evident that in the spatial case we have six degrees of freedom (excluding internal structure of the colliding particles), one of which is again taken as the energy. In Paper I it was demonstrated that (B) and (C) differed only by a (trivial) phase. As one may suspect, the relationship between

(B') and (C') is more complicated; in fact, they are connected by a unitary transformation whose elements are Clebsch-Gordon coefficients[6]

$$C^{\ell_1 \ell_2 L}_{m_1 m_2 M} \equiv \langle \ell_1 \ell_2 m_1 m_2 \,|\, L \ell_1 \ell_2 M \rangle$$

$$|\lambda L \ell_1 \ell_2 M\rangle = \sum_{\substack{m_1 m_2 \\ (m_1+m_2=M)}} |\lambda \ell_1 \ell_2 m_1 m_2\rangle\langle \ell_1 \ell_2 m_1 m_2 \,|\, L \ell_1 \ell_2 M\rangle \tag{1}$$

In Paper I we briefly discussed the physical significance of Λ^2 and the relationship of the generalized angular momentum variables to the criterion for a three-body collision in a plane. It was concluded that in the quantum regime the particles approach more closely as λ, the quantum number corresponding to Λ^2, decreases. For a given value of λ, the system most closely approaches a simultaneous collision of the three particles at vanishing σ (the eigenvalue of Σ_t) in the symmetric representation or at $\lambda = m_+$ in the asymmetric one. In the representation (C') the criterion for closest approach becomes $\lambda = \ell_1 + \ell_2$. It is intuitively obvious that larger values of λ will contribute to the three-body interactions when two-body lifetimes are long. The relationship can in fact be demonstrated, and Smith[7] has recently done this.

In most cases of interest, members of assemblies of particles interact with each other via two-body central forces, i.e., the direction of the forces is parallel to the line connecting the centers of the particles. If a third particle interacts with such a pair, a torque is exerted on the pair thereby changing its angular momentum. Hence $\lambda\ \ell_1 \ell_2 m_1 m_2$ are not "good quantum numbers" with respect to the interaction, and the computations of scattering amplitudes, phase shifts, etc., become extremely difficult to carry out. Some improvement is gained by the adoption of representation (B') since L^2 and L_z are rigorously conserved because of the absence of external forces. Actually it is easier to make the calculations using representation (C') and then transform to (B') with the aid of transformation (1). The coordinate system best suited to these representations is a hyperspherical one

$$
\begin{aligned}
\xi_1^1 &= \rho \cos\chi \sin\theta_1 \cos\phi_1 \\
\xi_2^1 &= \rho \cos\chi \sin\theta_1 \sin\phi_1 \\
\xi_3^1 &= \rho \cos\chi \cos\theta_1 \\
\xi_1^2 &= \rho \sin\chi \sin\theta_2 \cos\phi_2 \\
\xi_2^2 &= \rho \sin\chi \sin\theta_2 \sin\phi_2 \\
\xi_3^2 &= \rho \cos\chi \cos\theta_2
\end{aligned}
\qquad (2)
$$

in which we have used a spatial partitioning similar to that shown in Fig. 2 of Paper 1.

In two-particle scattering the two variables which are required to describe the kinematics of the elastic collision process are usually taken as the energy and the momentum transfer. In a three-body collision four variables are required to take account of the collision of the third particle with the 1-2 pair; generalizing to n-body collisions, we require 2(n-1) kinematic variables. In order to investigate the possible choices let us square the magnitude of the generalized momentum transfer using the coordinate system (2)

$$
\begin{aligned}
|\underset{\sim}{\Delta}|^2 \equiv |\underset{\sim}{\pi}^0 - \underset{\sim}{\pi}^i|^2 &= |\underset{\sim}{\pi}^0|^2 + |\underset{\sim}{\pi}^i|^2 - 2\underset{\sim}{\pi}^0\cdot\underset{\sim}{\pi}^i \\
&= |\underset{\sim}{\Delta}_\chi|^2 + |\underset{\sim}{\Delta}_1|^2 + |\underset{\sim}{\Delta}_2|^2
\end{aligned}
\qquad (3)
$$

where

$$|\underset{\sim}{\Delta}_1| = 2k \sin\tfrac{1}{2}(\theta_1{}^0 - \theta_1^i)(\cos\chi^0 \cos\chi^i)^{\frac{1}{2}}$$

$$|\underset{\sim}{\Delta}_2| = 2k \sin \tfrac{1}{2} (\theta_2^o - \theta_2^i)(\sin \chi^o \sin \chi^i)^{\frac{1}{2}} \tag{4}$$

$$|\underset{\sim}{\Delta}_\chi| = 2k \sin \tfrac{1}{2} (\chi^o - \chi^i)$$

and $|\underset{\sim}{\pi}^o| = |\underset{\sim}{\pi}^i| = k$ is the magnitude of the generalized momentum. The three quantities Δ_1, Δ_2, and Δ_χ have the following physical significance: Δ_1 is the momentum transfer between particles 1 and 2, Δ_2 is the momentum transfer between particle 3 and the 1-2 pair, and Δ_χ describes the change in "togetherness" (or "togetherness transfer") of the three particles brought about by the collision. The magnitudes of these three quantities, together with the energy $E = \frac{k^2}{2\mu}$, constitute a complete set of independent kinematic variables.

The Schrödinger equation describing the motion of the three particles can be written in terms of the variables $\underset{\sim}{\xi}^1$ and $\underset{\sim}{\xi}^2$ or alternatively in terms of the coordinates $(\rho, \chi, \theta_1, \theta_2, \phi_1, \phi_2)$. The former set yields plane wave solutions

$$< \underset{\sim}{\pi} | \underset{\sim}{\xi} > = \frac{1}{(2\pi)^3} \; e^{i\underset{\sim}{\pi} \cdot \underset{\sim}{\xi}} \tag{5}$$

in which we have chosen our units such that $\hbar = 1$ and the normalization is one particle per unit volume. In the absence of a potential the latter yield the solutions

$$< k\lambda \; \ell_1 \ell_2 m_1 m_2 | \rho\chi \; \theta_1\theta_2 \; \phi_1\phi_2 > = \frac{J_{\lambda+2}(k\rho)}{(k\rho)^2} \mathcal{L}_{\lambda\ell_1\ell_2 m_1 m_2}(\chi\theta_1\theta_2\phi_1\phi_2) \tag{6}$$

where $J_{\lambda+2}(k\rho)$ is the Bessel function of the first kind of order $\lambda+2$, k is the magnitude of the momentum $(k^2 = 2\mu K)$, and

$$\Lambda^2 \mathcal{L}_{\lambda\ell_1\ell_2 m_1 m_2} = \lambda(\lambda+4) \mathcal{L}_{\lambda\ell_1\ell_2 m_1 m_2} \tag{7a}$$

$$L^2_{1,2}\mathcal{L}_{\lambda\ell_1\ell_2m_1m_2} = \ell_{1,2}(\ell_{1,2}+1)\mathcal{L}_{\lambda\ell_1\ell_2m_1m_2} \tag{7b}$$

$$L_{1,2_z}\mathcal{L}_{\lambda\ell_1\ell_2m_1m_2} = m_{1,2}\mathcal{L}_{\lambda\ell_1\ell_2m_1m_2} \tag{7c}$$

$\mathcal{L}_{\lambda\ell_1\ell_2m_1m_2}(\chi,\theta_1,\theta_2,\phi_1,\phi_2)$ is given by[8]

$$\mathcal{L}_{\lambda,\ell_1\ell_2m_1m_2}(\chi,\theta_1,\theta_2,\phi_1,\phi_2) = N_{\lambda\ell_1\ell_2} \cos^{\ell_1}\chi \sin^{\ell_2}\chi$$

$$\times {}_2F_1[-\tfrac{1}{2}(\lambda-\ell_1-\ell_2),\ \tfrac{1}{2}(\lambda+\ell_1+\ell_2+4);\ \ \ell_2+\tfrac{3}{2};\ \sin^2\chi]$$

$$\times\ Y_{\ell_1m_1}(\theta_2,\phi_2)\ Y_{\ell_2m_2}(\theta_2,\phi_2) \tag{8a}$$

$$N^2_{\lambda\ell_1\ell_2} = \frac{2(\lambda+2)\Gamma[\frac{1}{2}(\lambda+\ell_1+\ell_2+4)]\ \Gamma[\frac{1}{2}(\lambda+\ell_1+\ell_2+3)]}{[\frac{1}{2}(\lambda-\ell_1-\ell_2)]!\,[\Gamma(\ell_2+\frac{3}{2})]^2\Gamma\ [\frac{1}{2}(\lambda\ell_1-\ell_2+3)]} \tag{8b}$$

where the ${}_2F_1(a,b;\ c;\ z)$ are Jacobi polynomials and the $Y_{\ell m}(\theta,\phi)$ are spherical harmonics.

In the following section we shall obtain the free-particle Green's function and equations for the scattering amplitude and cross section. Succeeding sections will deal with a three-body formulation of the optical theorem and with a simple application of the theory. Discussion of the analytic properties of the three-particle scattering amplitude will be reserved for a future paper.

II COLLISION DYNAMICS

As in Paper I, we write the equation for the state vector $|s\rangle$ of the system in integral form[2,3,4]

$$|s\rangle = |i\rangle + G^{(+)}(E_0)\ V\ |s\rangle \tag{9}$$

where $|i\rangle$ is the state vector at $t = -\infty$, V is the interaction potential, and $G^{(+)}(E_0)$ is a free-particle propagator

$$G^{(+)}(E_0) = \lim_{\epsilon \to +0} [E_0 - K + i\epsilon]^{-1} \tag{10}$$

In Eq. (10) K is the free-particle Hamiltonian operator and ϵ is the usual adiabatic switching parameter. In configuration space representation we thus have

$$\langle \underset{\sim}{\xi} | s\rangle = \langle \underset{\sim}{\xi} | i\rangle + \int G^{(+)}_{E_s}(\underset{\sim}{\xi},\underset{\sim}{\xi}')V(\underset{\sim}{\xi}')\langle \underset{\sim}{\xi}' | s\rangle \, d\underset{\sim}{\xi}' \tag{11}$$

where

$$G^{(+)}_{E_s}(\underset{\sim}{\xi},\underset{\sim}{\xi}') = \lim_{\epsilon \to +0} \frac{2\mu}{(2\pi)^6} \int \frac{e^{i\underset{\sim}{\pi}\cdot(\underset{\sim}{\xi}-\underset{\sim}{\xi}')}}{k_s^2 - k^2 + 2i\mu\epsilon} \, d\underset{\sim}{\pi} \; ; \; k = |\underset{\sim}{\pi}| \tag{12}$$

with the aid of some standard mathematical techniques[9] Eq. (12) can be cast in the form

$$G^{(+)}_{E_s}(\underset{\sim}{\xi},\underset{\sim}{\xi}') = \lim_{\epsilon \to +0} \frac{2\mu}{(2\pi)^6} \int_0^\infty \int_0^{\pi/2} \frac{J_{\frac{1}{2}}(k|\underset{\sim}{\xi}^1-\underset{\sim}{\xi}'^1|\cos\chi)J_{\frac{1}{2}}(k|\underset{\sim}{\xi}^2-\underset{\sim}{\xi}'^2|\sin\chi)}{|\underset{\sim}{\xi}^1-\underset{\sim}{\xi}'^1||\underset{\sim}{\xi}^2-\underset{\sim}{\xi}'^2|}$$

$$\times \sin^{\frac{3}{2}}\chi \cos^{\frac{3}{2}}\chi \frac{k^4}{k_s^2 - k^2 + 2i\mu\epsilon} \, d\chi dk$$

$$= \lim_{\epsilon \to +0} \frac{2\mu}{(2\pi)^3} \frac{1}{|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|^2} \int_0^\infty \frac{J_2(k|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|)}{k_s^2 - k^2 + 2i\mu\epsilon} \, k^3 dk \tag{13}$$

The integration indicated in Eq. (13) is carried out over contours around the first and fourth quadrants (see Paper I), yielding

$$G^{(+)}_{E_s}(\underset{\sim}{\xi},\underset{\sim}{\xi}') = \frac{\mu i}{(8\pi)^2} \; k_s^2\left(\frac{1}{|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|}\frac{\partial}{\partial|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|}\right)^2 H_0^{(1)}(k|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|)$$

$$= \frac{\mu i}{(8\pi)^2} \frac{k_s^2}{|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|^2} \; H_2^{(1)}(k|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|) \tag{14}$$

which takes the asymptotic form

$$G_{E_s}^{(+)}(\underset{\sim}{\xi},\underset{\sim}{\xi}') = \frac{\mu}{(2\pi)^{5/2}} \frac{k_s^{3/2}}{|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|^{5/2}} e^{-\frac{3}{4}\pi i} e^{ik|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|}. \tag{15}$$

One can also express the Green's function in terms of the hyperspherical wave functions (6) in which case we obtain

$$G_{E_s}^{(+)}(\underset{\sim}{\xi},\underset{\sim}{\xi}^1) = \pi i\mu \sum_{\alpha} \mathcal{L}_\alpha(\hat{\xi})\mathcal{L}_\alpha^*(\hat{\xi}') \frac{H_{\lambda+2}^{(1)}(k\rho)J_{\lambda+2}(k\rho')}{\rho^2\rho'^2} \quad , \rho > \rho' \tag{16}$$

where α denotes the set of quantum numbers $\lambda\ell_1\ell_2 m_1 m_2$.

Inelastic scattering is possible if one or more of the particles has internal structure. If all three are of this type, the free-particle wave functions can be written

$$\phi_i = \frac{1}{(2\pi)^3} R_m(\rho)S_n(\sigma)T_p(\tau) \exp\left[i(\underset{\sim}{\pi}_\alpha^1 \cdot \underset{\sim}{\xi}^1 + \underset{\sim}{\pi}_\alpha^2 \cdot \underset{\sim}{\xi}^2)\right] \tag{17}$$

where $R_n(\rho)$, $S_n(\sigma)$, and $T_\rho(\tau)$ represent the internal wave functions of the particles. The Green's function (12) of the interaction then takes the form

$$G_E^{(+)}(\underset{\sim}{\xi},\underset{\sim}{\xi}') = \lim_{\epsilon\to+0} \frac{1}{(2\pi)^6} \sum_{\mu\nu\lambda} \int \frac{\exp[i\,\underset{\sim}{\pi}_\alpha \cdot (\underset{\sim}{\xi}-\underset{\sim}{\xi}')]}{E-E_\alpha-E_\lambda-E_\nu-E_\mu+i\epsilon}$$

$$\times\, R_\mu(\rho)S_\nu(\sigma)T_\lambda(\tau)R_\mu^*(\rho')S_\nu^*(\sigma')T_\lambda^*(\tau')\, d\underset{\sim}{\pi}_\alpha \tag{18}$$

When the integration is performed as in Paper I, we obtain

$$G_E^{(+)}(\underset{\sim}{\xi}\rho\sigma\tau;\ \underset{\sim}{\xi}'\rho'\sigma'\tau') = \sum_{\mu\nu\lambda} \frac{i\mu k_{\mu\nu\lambda} H_2^{(1)}(k_{\mu\nu\lambda}|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|)}{|\underset{\sim}{\xi} - \underset{\sim}{\xi}'|^2}$$

$$\times\, R_\mu(\rho)S_\nu(\sigma)T_\lambda(\tau)R_\mu^*(\rho')S_\nu^*(\sigma')T_\lambda^*(\tau') \tag{19}$$

in which we have made the replacement

$$(\frac{1}{2\mu})k^2_{\mu\nu\lambda} = E - E_\lambda - E_\nu - E_\mu \cdot \tag{20}$$

Expressed in terms of the generalized angular momentum eigenfunctions (representation C') Eq. (19) becomes

$$G_E^{(+)}(\underset{\sim}{\xi}\rho\sigma\tau;\ \underset{\sim}{\xi}'\rho'\sigma'\tau') = i\mu \sum_{\mu\nu\lambda} \sum_{\alpha} \mathscr{L}_\alpha(\hat{\xi})\mathscr{L}^*_\alpha(\hat{\xi}')$$

$$\times \frac{H^{(1)}_{\lambda+2}(k_{\mu\nu\lambda}\rho)J_{\lambda+2}(k_{\mu\nu\lambda}\rho')}{\rho^2\rho'^2} R_\mu(\rho)S_\nu(\sigma)T_\lambda(\tau)R_\mu{}^*(\rho')S^*_\nu(\sigma')T^*_\lambda(\tau') \tag{21}$$

This form can easily be recast in representation (B') with the aid of the unitary transformation (1).

With the aid of an elementary extension of the methods employed in Appendix A of Paper I we can readily obtain the N-body Green's functions for elastic scattering. As one may suspect the results for odd-N and even-N are different:

$$G_E^{(+)}(\underset{\sim}{\xi},\underset{\sim}{\xi}') = \frac{\pi\mu i}{(2\pi)^{(3/2)(N-1)}}\left(-\frac{1}{|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|}\frac{\partial}{\partial|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|}\right)^{N-1} H_0{}^{(1)}(k|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|) \quad \text{(odd N)}$$

$$G_E^{(+)}(\underset{\sim}{\xi},\underset{\sim}{\xi}') = \frac{\mu k}{2(2\pi)^{(3/2)(N-1)-1}}\left(\frac{1}{|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|}\frac{\partial}{\partial|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|}\right)^{N-2}\left[\frac{H_{\frac{1}{2}}{}^{(1)}(k|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|)}{(k|\underset{\sim}{\xi}-\underset{\sim}{\xi}'|)^{\frac{1}{2}}}\right] \quad \text{(even N)}$$

(22)

Although Eq. (22) will not be used again in this paper, it is an interesting generalization of the methods employed here.

The asymptotic form of the wave function (11) can be expressed in terms of a scattering amplitude $f(\hat{\pi}_i,\hat{\pi}_0)$:

$$\psi_{\underset{\sim}{\pi}_i}(\underset{\sim}{\xi}) = \phi_{\underset{\sim}{\pi}_i}(\underset{\sim}{\xi}) + \frac{k^{3/2} e^{-\frac{3}{4}\pi i}}{\rho^{5/2}} e^{ik\rho} f(\hat{\pi}_0, \hat{\pi}_i) \tag{23}$$

which is related to the cross section, where

$$f(\hat{\pi}_0, \hat{\pi}_i) = \frac{\mu}{(2\pi)^{5/2}} \int e^{-ik\rho\hat{\xi}\cdot\hat{\xi}'} V(\underset{\sim}{\xi}') \, \psi_{\underset{\sim}{\pi}_i}(\underset{\sim}{\xi}') d\underset{\sim}{\xi}', \tag{24}$$

and $\hat{\pi}_0$ and $\hat{\pi}_i$ represent the directions of the incoming and scattered three-particle momenta, respectively. As we saw in Paper I, it is frequently more useful to expand the scattering amplitude in a series of generalized angular momentum eigenfunctions:

$$f(\hat{\pi}_0, \hat{\pi}_i) = \sum_{\substack{\lambda \ell_1 \ell_2 m_1 m_2 \\ \lambda' \ell_1' \ell_2' m_1' m_2'}} \mathcal{L}^*_{\lambda \ell_1 \ell_2 m_1 m_2}(\hat{\pi}_0) \, f^{\lambda' \ell_1' \ell_2' m_1' m_2'}_{\lambda \ell_1 \ell_2 m_1 m_2} \, \mathcal{L}_{\lambda \ell_1' \ell_2' m_1' m_2'}(\hat{\pi}_i) \tag{25}$$

where

$$f^{\lambda \ell_1' \ell_2' m_1' m_2'}_{\lambda \ell_1 \ell_2 m_1 m_2} = (2\pi)^{1/2} \frac{\mu}{k^2} (-i)^{\lambda} \int \frac{J_{\lambda+2}(k\rho)}{\rho^2} \mathcal{L}^*_{\lambda \ell_1 \ell_2 m_1 m_2}(\hat{\xi}) \, V(\underset{\sim}{\xi}) \psi_{\lambda' \ell_1' \ell_2' m_1' m_2'}(\underset{\sim}{\xi}) d\underset{\sim}{\xi} \tag{26}$$

In the earlier work the relationship of the scattering amplitude to the three-body differential cross section $\sigma(\underset{\sim}{\pi}_i, \underset{\sim}{\pi}_0)$ was developed in two different ways. The first proceeded from the ratio between the magnitude of the scattered flux and the incoming current density, whereas the second approach was via time-dependent perturbation theory which gives the cross section in terms of a transition matrix element $R_{\underset{\sim}{\pi}^0, \underset{\sim}{\pi}^i}$

$$\sigma(\underset{\sim}{\pi}_0, \underset{\sim}{\pi}_i) = \frac{2\pi}{v_0} \rho(E) |R_{\underset{\sim}{\pi}_0, \underset{\sim}{\pi}_i}|^2; \tag{27}$$

v_0 is the velocity of the incoming particles given by $v_0 = k/\mu$, $\rho(E)$ is the number of final states per unit energy, and[4]

$$R_{\underset{\sim}{\pi}_0,\underset{\sim}{\pi}_i} = \lim_{\epsilon \to +0} - i\epsilon < \underset{\sim}{\pi}_0 | \underset{\sim}{\pi}_i > \tag{28}$$

Both schemes, of course, yield the same result,

$$\sigma(\underset{\sim}{\pi}_0,\underset{\sim}{\pi}_i) = k^3 |f(\hat{\pi}_0,\hat{\pi}_i)|^2 \tag{29}$$

for elastic collisions, and

$$\sigma(\underset{\sim}{\pi}_0,\underset{\sim}{\pi}_i) = \frac{k_0^4}{k_i} |f(\hat{\pi}_0,\hat{\pi}_i)|^2 . \tag{30}$$

for inelastic collisions. The total cross section is obtained by integrating $\sigma(\underset{\sim}{\pi}_0,\underset{\sim}{\pi}_i)$ over the hypersolid angle Ω where

$$d\Omega = \sin^2 \chi \cos^2 \chi \, d\chi \, \sin \theta_1 d\theta_1 \, \sin\theta_2 d\theta_2 d\phi_1 d\phi_2 \ . \tag{31}$$

Substitution of the expansion (25) for $f(\hat{\pi}_0,\hat{\pi}_i)$ into Eq. (29) yields

$$\sigma = k^3 \sum_{\alpha\alpha'} | f_\alpha^{\alpha'} |^2 \tag{32}$$

where α represents the quantum numbers $\lambda\ell_1\ell_2 m_1 m_2$. Thus the cross section for scattering from the set $(\lambda\ell_1\ell_2 m_1 m_2)$ to the set $(\lambda\ell_1' m_1' m_2')$ is

$$\sigma_k(\alpha \to \alpha') = k^3 |f_\alpha^{\alpha'}|^2 \tag{33}$$

Physically, the cross section σ has the significance of a two-body collision cross section of, for example, particles 1 and 2 multiplied by the volume within which the third particle must lie in order that two-particle interactions occur simultaneously.

In the same way as in Paper I we can introduce a three-particle scattering matrix $S_{\alpha\alpha'}$, which connects the exit and entrance channels, specified, for example, by the sets of quantum numbers α, α'. The cross section $\sigma_k(\alpha \to \alpha')$ is related to $S_{\alpha\alpha'}$ by

$$\sigma_k\ (\alpha \to \alpha') = (\frac{2\pi}{k})^5 \left|\delta_{\alpha\alpha'} - S_{\alpha\alpha'}\right|^2 \ ; \tag{34}$$

Comparison of Eqs. (33) and (34) immediately leads to the following relationship between the scattering matrix and the scattering amplitude

$$S_{\alpha\alpha'} = \delta_{\alpha\alpha'} - \frac{k^4}{(2\pi)^{5/2}} f_{\alpha}^{\alpha'} \ . \tag{35}$$

In order to gain further insight into the physics of the collision process it is convenient to expand the state vector given by Eq. (9) in a Born series

$$|s\rangle = |i\rangle + GV|i\rangle + GVGV|i\rangle + \ldots . \tag{36}$$

If $V(\xi)$ is written as the sum of three two-particle potentials and the result inserted in Eq. (36), we see immediately that $|s\rangle$ contains contributions from two-particle (pseudo three-particle) as well as from three-particle collisions. The two-body contributions arise from the second term in the Born series and also from higher order terms like $GV_{12}GV_{12}|i\rangle$. One can, in fact, construct scattering diagrams corresponding to each such term in the series and this is illustrated in Fig. 1. As an example of the two-body contributions, it is instructive to evaluate the scattering amplitude in first Born approximation due to the potential V_{12} acting between particles 1 and 2. From Eq. (24) we obtain

$$f(\hat{\pi}^0, \hat{\pi}^1) = \frac{\mu}{(2\pi)^{3/2}} \delta(\underset{\sim}{\pi}_i^2 - \underset{\sim}{\pi}_0^2) \int V_{12}(\underset{\sim}{\xi}^i) e^{i(\underset{\sim}{\pi}_i^1 - \underset{\sim}{\pi}_1^1)\cdot\underset{\sim}{\xi}^1} d\underset{\sim}{\xi}^1 \tag{37}$$

which is a divergent as a result of the delta function. Integration over $\underset{\sim}{\pi}_i^2$ yields a finite result which is merely the uninteresting two-body scattering amplitude of particles 1 and 2. Hence, the second term in the series will not contribute to the three-body scattering amplitude when the interactions are of the two-body type. If, however, the wave function appearing under the integral of Eq. (11) is represented by an appropriately distorted wave, the term corresponding to $GV|i\rangle$ does in fact yield three-body contributions; for example, $V_{23}(\underset{\sim}{\xi})$ contributes to the term containing $V_{12}(\underset{\sim}{\xi})$ by distorting the approximate wave function used in the integral expression for the scattering amplitude. The exclusion of two-body contributions was not discussed in Paper I.

Of great interest in any discussion of three-body scattering are rearrangement collisions[10,11,12] which are subject to the usual difficulties inherent in the quantum mechanical treatment of processes of this type: nonorthogonality of the initial and final states and inapplicability of perturbation theory in cases where the interaction can not be treated as small.[12] If computations could be carried out exactly, the first difficulty would not arise; it is introduced by the necessity for making approximations in order to render the mathematics tractable. Mittleman[12] has developed a formal approach which avoids this ambiguity by reformulating the transition amplitude so that it contains transitions only between mutually orthogonal states.

As an example of a three-body rearrangement collision it is instructive to investigate the case of two-particle combination

$$A + B + C \rightarrow A + BC \tag{38}$$

In Paper I we showed that we could employ the so-called "prior interaction" (i.e., that in which the three interacting particles are unbound)

$$V_i = V^0_{A,B,C} \tag{39}$$

to obtain the scattering amplitude in a form similar to that resulting from use of the "post interaction" (i.e., that in which two of the particles are bound)

$$V_f = V_{A,BC} \tag{40}$$

where

$$H_i + V_i = H_f + V_f \tag{41}$$

and H_i, H_f are the non-interacting Hamiltonians.

This was approached by introducing a complex χ

$$\chi = \frac{\pi}{2} + i\alpha$$

into the equation for the Green's function, Eq. (19). The same method can be readily applied to three-particle scattering in space, yielding

$$\psi_{\underset{\sim}{\pi}_i}(\underset{\sim}{\xi}) = \sum_n \frac{e^{ik_n}}{\xi^2} \phi_n(\underset{\sim}{\xi}^1)\ f(\hat{\pi}^o_{2n}, \hat{\pi}^i_{2n}) \tag{42}$$

where $\phi_n(\underset{\sim}{\xi}^1)$ is the internal wave function of the "molecule" BC with internal coordinates $\underset{\sim}{\xi}^1$ and binding energy

$$E^n_{BC} = -\frac{1}{2\mu} k^2 \sinh^2 \alpha_n, \tag{43}$$

k_n is the relative momentum of A and BC

$$k_n = 2\mu(E^{in} - E^n_{BC})^{1/2} \tag{44}$$

and $f(\hat{\pi}^o_{2n}, \hat{\pi}^i_{2n})$ is the two-body scattering amplitude written in the "prior-interaction" form

$$f(\hat{\pi}^o_{2n}, \hat{\pi}^i_{2n}) = \frac{\mu}{2\pi} \int e^{-i\underset{\sim}{\pi}_{2n}\cdot\underset{\sim}{\xi}_2} \phi_n(\underset{\sim}{\xi}_1) V_{A,B,C}(\underset{\sim}{\xi}) \psi_{\pi_i}(\underset{\sim}{\xi}) d\underset{\sim}{\xi} \tag{45}$$

which is formally similar to the "post-interaction" amplitude

$$f(\hat{\pi}^0,\hat{\pi}^i) = \frac{\mu}{2\pi}\int e^{-i\pi_2\cdot\xi} V_{A,BC}(\xi)\psi_{\pi_0}(\xi)d\xi \tag{46}$$

In practical problems such as three-body recombination of atoms or three-body electron attachment form (46) is expected to be more tractable than (45). We are of course still faced with the second difficulty mentioned above, i.e., the interaction potential can not be justifiably treated as small.

Variational methods such as those of Hulthén and Kohn and of Schwinger[13] can easily be adapted to the three-body problem. Schwinger's approach which was discussed briefly in Paper I proceeds via an integral expression for the scattering amplitude

$$f(\hat{\pi}_0,\hat{\pi}_i) = \frac{[\int \psi^*(\xi)\, U(\xi)\, e^{i\pi_i\cdot\xi}d\xi][\int e^{-i\pi_0\cdot\xi}\, U(\xi')\psi(\xi')d\xi']}{[\int \psi^*(\xi)\, U(\xi)\psi(\xi)d\xi \int\int \psi^*(\xi)\, U(\xi)\, G(\xi,\xi')\, U(\xi')\psi(\xi')d\xi' d\xi']} \tag{47}$$

in which $U(\xi) = 2\mu V(\xi)$. When f is varied with respect to ψ^*, Eq. (24) results. In order to apply this technique one can, for example, expand ψ as a linear combination of a suitable set of functions and vary the scattering amplitude with regard to the expansion coefficients. If a judicious choice of expansion functions has been made, the computed value of f should be close to the true one. By contrast Hulthén's variational principle[13] involves the use of differential rather than integral forms to construct a functional which is varied subject to the appropriate boundary conditions. Actually the functionals proposed by Schwinger and Hulthén apparently do not always satisfy the appropriate boundary condition (<u>outgoing</u> scattered waves) for approximate wave functions. Malik[14,15] has shown how the functional can be modified in such a way that this difficulty is avoided.

III OPTICAL THEOREM

In two-particle scattering one can obtain a relation between the total cross section and the scattering amplitude corresponding to the forward direction. This is a consequence of the conservation of particles, or equivalently, of the unitarity of the scattering operator, $S^{\dagger}S = 1$. The extension to the three-particle case is simple. We begin by writing S as the sum of the unit operator and a transition operator T :

$$S = 1 + T \tag{48}$$

Then we obviously have

$$T^{*} T = -(T + T^{*}) = -2\mathrm{Re}T \tag{49}$$

or in matrix representation

$$-2\mathrm{Re} \langle f|T|i\rangle = \sum_{m} \left|\langle f|T|i\rangle\right|^{2} . \tag{50}$$

The transition matrix elements are related to the scattering amplitude $f(\hat{\pi}^{m}, \hat{\pi}^{i})$ by the equality

$$f(\hat{\pi}^{m}, \hat{\pi}^{i}) = \frac{\mu i}{(2\pi)^{5/2}} \delta(E_{m} - E_{i}) \langle f|T|i\rangle. \tag{51}$$

Substitution of Eq. (51) into (50) yields

$$2(2\pi)^{5/2} \text{ Im } f(\hat{\pi}^{f}, \hat{\pi}^{i}) = k^{4} \int f^{*}(\hat{\pi}^{m}, \hat{\pi}^{f})\, f(\hat{\pi}^{m}, \hat{\pi}^{i})\, d\hat{\pi}^{m} \tag{52}$$

which is the desired statement of the optical theorem. Since the three-body cross section σ is related to the scattering amplitude by

$$\sigma = k^{3} \int \left|f(\hat{\pi}^{f}, \hat{\pi}^{i})\right|^{2} d\,\hat{\pi}f, \tag{53}$$

we can write the following relationship between the cross section and the "forward" scattering amplitude $f(\hat{\pi}^i, \hat{\pi}^i)$

$$\frac{2(2\pi)^{5/2}}{k} \operatorname{Im} f(\hat{\pi}^i, \hat{\pi}^i) = \sigma \tag{54}$$

which is the same expression one obtains for two-body scattering to within a factor of $(2\pi)^{3/2}$.

IV APPLICATION

To illustrate the methods developed in Section II for the computation of the three-particle scattering cross section, we shall treat briefly the case of interaction via short range two-body central potentials which for simplicity will be chosen to be of the well-type

$$\begin{aligned} V(r_{ij}) &= V_0 \text{ if} |\underset{\sim}{x}^j - \underset{\sim}{x}^i| \leq a \\ &= 0 \text{ if} |\underset{\sim}{x}^j - \underset{\sim}{x}^i| > a \quad . \end{aligned} \tag{55}$$

Although particles will be assumed to be identical, the antisymmetrization requirement on the wave function will be omitted, again for the sake of simplicity. Expressing Eq. (55) in the coordinate system specified by Eq. (2) of Paper I

$$\begin{aligned} \underset{\sim}{x}^2 - \underset{\sim}{x}^1 &= d\underset{\sim}{\xi}^1 \\ \underset{\sim}{x}^3 - \underset{\sim}{x}^1 &= \frac{1}{d}\underset{\sim}{\xi}^2 + \frac{d}{2}\underset{\sim}{\xi}^1 \\ \underset{\sim}{x}^3 - \underset{\sim}{x}^2 &= \frac{1}{d}\underset{\sim}{\xi}^2 - \frac{d}{2}\underset{\sim}{\xi}^1 \end{aligned} \tag{56}$$

and Eq. (2) of this paper, we obtain

$$\begin{aligned} V(r_{12}) &= V_0 \text{ if } \rho \cos \chi \leq \frac{a}{d} \\ &= 0 \text{ if } \rho \cos \chi > \frac{a}{d} \end{aligned} \tag{57}$$

$$V(r_{13}) = V_0 \text{ if } \rho[(\frac{d}{2}\cos\chi)^2 + (\frac{1}{d}\sin\chi)^2 - \sin\chi\cos\chi\cos\omega]^{1/2} \leq a$$

$$= 0 \text{ if } \rho[(\frac{d}{2}\cos\chi)^2 + (\frac{1}{d}\sin\chi)^2 - \sin\chi\cos\chi\cos\omega]^{1/2} > a$$

$$V(r_{13}) = V_0 \text{ if } \rho[(\frac{d}{2}\cos\chi)^2 + (\frac{1}{d}\sin\chi)^2 + \sin\chi\cos\chi\cos\omega]^{1/2} \leq a$$

$$= 0 \text{ if } \rho[(\frac{d}{2}\cos\chi)^2 + (\frac{1}{d}\sin\chi)^2 + \sin\chi\cos\chi\cos\omega]^{1/2} > a$$

where $\cos\omega = \hat{\xi}^1 \cdot \hat{\xi}^2$.

If we now insert the potential specified by Eq. (57) into the three-body Schrödinger equation, multiply by $\mathcal{L}_\alpha^* (\hat{\xi})$, and integrate over the hypersolid angle Ω, we obtain a series of coupled radial equations

$$\frac{1}{\rho^5}\frac{d}{d\rho}(\rho^5 \frac{dR_{\alpha\alpha''}}{d\rho}) + (k^2 - \frac{\lambda(\lambda+4)}{\rho^2})R_{\alpha\alpha''} - 2\mu\sum_{\alpha'} v_{\alpha\alpha'} R_{\alpha'\alpha''} = 0 \qquad (58)$$

in which

$$v_{\alpha\alpha'}(\rho) = V_0[\int_A \mathcal{L}_\alpha^* (\hat{\xi})\mathcal{L}_{\alpha'}(\hat{\xi})d\Omega + \int_B \mathcal{L}_\alpha^* (\hat{\xi})\mathcal{L}_{\alpha'}(\hat{\xi})d\Omega + \int_C \mathcal{L}_\alpha^* (\hat{\xi})\mathcal{L}_{\alpha'}(\hat{\xi})d\Omega] \quad (58.)$$

are the transformed potentials; A, B, and C refer to the constraints specified in Eq. (57). Clearly the potential matrix whose elements are $v_{\alpha\alpha'}$ is not diagonal because of the "non-central" character of the constraints (57).

The asymptotic solution to the radial equation (58) in the absence of interaction is

$$R_{\alpha\alpha'} \sim \frac{2}{\sqrt{2\pi}}\frac{1}{(k\rho)^{5/2}} \sin\,(k\rho - \frac{2\lambda+3}{4}\pi)\delta_{\alpha\alpha'} \qquad (60)$$

Since the potential falls off faster than ρ^{-2}, the effect of the interaction is to introduce a (non-diagonal) phase shift $\eta_{\alpha\alpha'}$. The complete asymptotic wave function with interaction is thus

$$\psi_{\underset{\sim}{\pi} i}(\underset{\sim}{\xi}) \sim \left(\frac{2}{\pi}\right)^{1/2} \sum_{\alpha\alpha'\alpha''} (i)^{\lambda} \frac{\sin\left(k\rho \frac{2\lambda+3}{4}\pi + \eta_{\alpha\alpha'}\right)}{(k\rho)^{5/2}} A_{\alpha'\alpha''} \mathcal{L}^{*}_{\alpha}(\hat{\pi}^{i}) \mathcal{L}_{\alpha''}(\hat{\xi}) \quad (61)$$

Substitution into Eq. (23) of the form of $\psi_{\underset{\sim}{\pi} i}$ given by Eq. (61), together with the expansion of the plane wave $e^{i\underset{\sim}{\pi}\cdot\underset{\sim}{\xi}}$ in eigenfunctions of the three-body Schrödinger equation without interaction,

$$e^{i\underset{\sim}{\pi}\cdot\underset{\sim}{\xi}} = (2\pi)^3 \sum_{\alpha} (i)^{\lambda} \frac{J_{\lambda+2}(k\rho)}{(k\rho)^2} \mathcal{L}^{*}_{\alpha}(\hat{\pi}) \mathcal{L}_{\alpha}(\hat{\xi}) \; , \qquad (62)$$

enables us to evaluate the scattering amplitude in terms of the phase shifts $\eta_{\alpha\alpha'}$. We then compare the incident wave terms which appear on the right and left hand sides of the equation in order to obtain the following relationship (in matrix notation) of $A_{\alpha\alpha'}$ to $\eta_{\alpha\alpha'}$

$$\mathbf{A} = (2\pi)^3 \, e^{i\boldsymbol{\eta}} \qquad (63)$$

Clearly the phase shifts $\eta_{\alpha\alpha'}$ are related to the scattering amplitude by

$$f = \frac{(2\pi)^{5/2}}{ik^4} \left(e^{2i\boldsymbol{\eta}} - 1\right) \qquad (64)$$

and to the scattering matrix S by

$$S = e^{2i\boldsymbol{\eta}} \qquad (65)$$

The scattering amplitudes and thus the phase shifts can be evaluated from the interaction potential by means of suitable approximations, e.g., the second Born approximation. This approach yields the following expression for the scattering amplitude

$$f_{\alpha}^{\alpha''} = \frac{\mu^2}{2k^4} (2\pi)^{9/2} (i)^{\lambda'' - \lambda + 2} \sum_{i<h;j} \sum_{\alpha'} \int_{\rho'>\rho''} J_{\lambda+2}(k\rho') v^{ij}_{\alpha\alpha'}(\rho')$$

$$\times\, H_{\lambda'+2}(k\rho')\rho' d\rho' \int J_{\lambda'+2}(k\rho'')\, V^{jk}_{\alpha'\alpha''}(\rho'')\, J_{\lambda''+2}(k\rho'')\rho''^{3} d\rho'' \qquad (66)$$

which can be readily computed from the information concerning the potential given previously. However, the required integrations can only be performed numerically and we shall not attempt this here. In place of the Born approximation one of the variational techniques described in Section II could also be employed, expanding the wave function $\psi_{\underline{\Pi} i}$ in a suitable set of trial functions or otherwise writing it as a function of a set of variation parameters. In computing the collision cross section, we must of course exclude the spurious contributions corresponding to purely two-body collisions.

APPENDIX

PLANE WAVE EXPANSION

We wish to expand the plane wave exp $(i\underset{\sim}{\pi} \cdot \underset{\sim}{\xi})$ in hyperradial and angular momentum eigenfunctions. This is facilitated by writing the plane wave as a product of two plane waves in the spaces of $\underset{\sim}{\xi}^1$ and of $\underset{\sim}{\xi}^2$, respectively:

$$e^{i\underset{\sim}{\pi}\cdot\underset{\sim}{\xi}} \equiv e^{i(\underset{\sim}{\pi}^1\cdot\underset{\sim}{\xi}^1 + \underset{\sim}{\pi}^2\cdot\underset{\sim}{\xi}^2)} = e^{i\underset{\sim}{\pi}^1\cdot\underset{\sim}{\xi}^1}\, e^{i\underset{\sim}{\pi}^2\cdot\underset{\sim}{\xi}^2} \tag{A1}$$

Each of the plane waves in the product is expanded in a series of Bessel functions and spherical harmonics and the series are then multiplied term by term

$$e^{i\underset{\sim}{\pi}\cdot\underset{\sim}{\xi}} = (2\pi)^3 \sum_{\ell_1 m_1} \sum_{\ell_2 m_2} (i)^{\ell_1+\ell_2} \frac{J_{\ell_1+\frac{1}{2}}(k\rho \cos\chi \cos\bar{\chi}) J_{\ell_2+\frac{1}{2}}(k\rho \sin\chi \sin\bar{\chi})}{k\rho(\cos\chi \cos\bar{\chi} \sin\chi \sin\bar{\chi})^{\frac{1}{2}}}$$

$$\times\, Y^*_{\ell_1 m_1}(\hat{\pi}^1) Y_{\ell_1 m_1}(\hat{\xi}^1)\, Y^*_{\ell_2 m_2}(\hat{\pi}^2)\, Y^*_{\ell_2 m_2}(\hat{\xi}^2), \tag{A2}$$

where $\underset{\sim}{\pi}^1\cdot\underset{\sim}{\xi}^1 = k\rho \cos\chi \cos\bar{\chi}(\hat{\pi}^1\cdot\hat{\xi}^1)$ and $\underset{\sim}{\pi}^2\cdot\underset{\sim}{\xi}^2 = k\rho \sin\chi \sin\bar{\chi}(\hat{\pi}^2\cdot\hat{\xi}^2)$. Using a well-known therorem for the addition of Bessel functions[9]

$$J_{\ell+\frac{1}{2}}(k\rho \cos\chi \cos\bar{\chi})\, J_{\ell+\frac{1}{2}}(k\rho \sin\chi \sin\bar{\chi}) = \sum_{\lambda=0}^{\infty} (-1)^\lambda \frac{J_{\ell_1+\ell_2+2+2+2\lambda}(k\rho)}{k\rho}$$

$$\times \cos^{\ell_1+\frac{1}{2}}\chi \sin^{\ell_2+\frac{1}{2}}\chi \quad \cos^{\ell_1+\frac{1}{2}}\bar{\chi} \sin^{\ell_2+}\bar{\chi}\ {}_2F^1(-\lambda_1, \ell_1+\ell_2+\lambda+ 2; \ell_2+\tfrac{3}{2}; \sin^2\chi)$$

$$\times\ {}_2F^1(-\lambda, \ell_1+\ell_2+\lambda+2; \ell_2+\tfrac{3}{2}; \sin^2\bar{\chi}) \frac{(\lambda+\ell_1+\ell_2+1)!\,(\lambda+\ell_2+\frac{1}{2})!\,2(\ell_1+\ell_2+2\lambda+2)}{\lambda!(\lambda+\ell_1+\frac{1}{2})!\ [(\ell_2+\frac{1}{2})!]^2}, \tag{A3}$$

we can rewrite Eq. (A2) as

$$e^{i\underset{\sim}{\pi}\cdot\underset{\sim}{\xi}} = (2\pi)^3 \sum_{\lambda\ \ell_1\ell_2 m_1 m_2} (i)^\lambda \frac{J_{\lambda+2}}{(k\rho)^2} \mathcal{L}^*_{\lambda\ell_1\ell_2 m_1 m_2}(\hat{\pi})\, \mathcal{L}_{\lambda\ell_1\ell_2 m_1 m_2}(\hat{\xi}) \qquad \text{(A4)}$$

after making the replacement $\lambda \to \frac{1}{2}(\lambda-\ell_1-\ell_2)$. The same method could have been used to obtain the plane wave expansion developed in Appendix B of Paper I.

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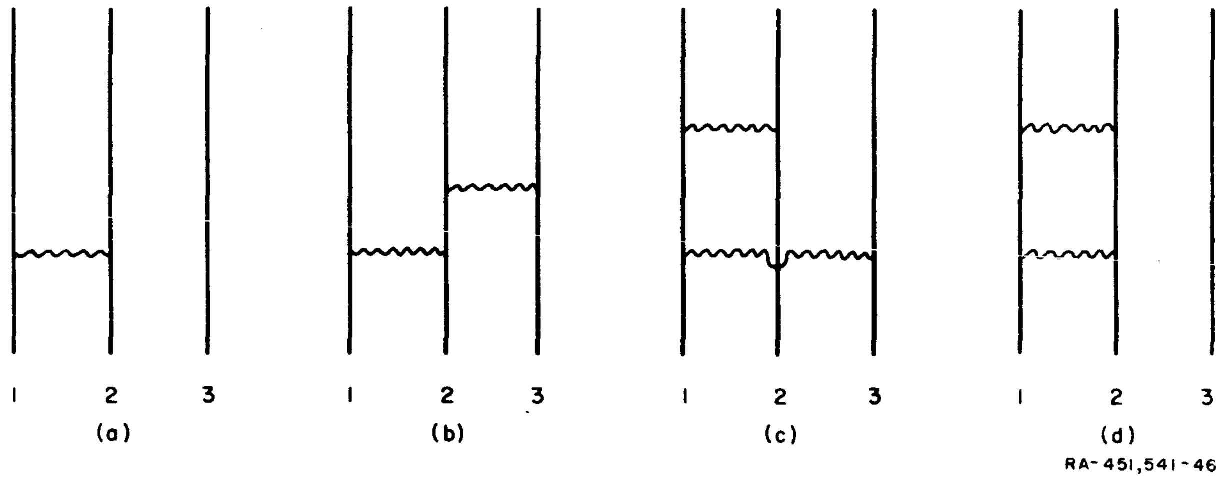

FIG. 1 THREE-BODY SCATTERING DIAGRAMS. (a) DIAGRAM CORRESPONDING TO THE FIRST-ORDER TERM IN THE BORN SERIES WHICH CONTAINS THE INTERACTION V_{12}. THIS PSEUDO THREE-BODY PROCESS IS REPRESENTED BY THE AMPLITUDE GIVEN IN EQ. (37). (b) AND (c) DIAGRAMS CORRESPONDING TO THE SECOND ORDER TERM IN THE BORN SERIES WHICH CONTAIN $V_{12}V_{23}$ AND $V_{13}V_{12}$, RESPECTIVELY. (d) PSEUDO THREE-BODY DIAGRAM CORRESPONDING TO THE SECOND ORDER TERM IN THE BORN SERIES WHICH CONTAINS $V_{12}V_{12}$.